J. Fac. Appl. Biol. Sci.,
Hiroshima Univ. (1979), **18**: 171－184

Inference of the Pseudo Transforming Mechanisms of Foods used a Simple Rate Equation

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Received Sept. 12, 1979
(Figs. 1–4, Tables 1–2)

INTRODUCTION

In order to design and to control various food transforming apparatuses, it is necessary to determine a excellent rate equation from the experimental rate data. Because most of the foods have complicated components and configurations, their real transforming mechanisms could not be elucidated thoroughly. Then the determination of the simple empirical rate equation has been investigated in a previous paper[1].

To obtain the theoretical rate equation which is better than the simple empirical one, we must elucidate minutely the transforming mechanisms taking as basis the calculation of various assumed rate equation. In this paper, we investigated the inference of the pseudo transforming mechanisms of foods by using a simple empirical rate equation proposed already in the previous paper. The pseudo mechanism infered in this paper is very efficient for finding the real mechanism.

SIMPLE RATE EQUATIONS

Most of the transforming mechanisms of food are in reality complicated. Therefore, we first assume some simple transforming mechanisms which give us a simple pseudo transforming mechanism and its simple rate equation.

1. *n*th-order rate equation

When the chemical and biological transformations are complicated, and we can not elucidate the real mechanisms, the over-all rate equation is usually expressed by the *n*th-order reaction rate equation as follows:

$$\text{A (main reactant)} \xrightarrow{k_r} \text{B (main product)} \tag{1}$$

$$-dC_A/d\theta = k_r(C_A - C_{Ae})^n \tag{2}$$

where, C_A (g-mol/cm^3) is the concentration of a main reacition component A at reaction time θ (min), and C_{Ae} is the equilibrium one. k_r (cm$^{3(n-1)}$ · g-mol^{1-n}· min^{-1}) and n(−) are the rate parameters which can be obtained from the experimental data.

Then, using a transforming ratio x_A (−) expressed by Eq. (3), the rate equation is

expressed as follows:

$$x_A = (C_{AO} - C_A)/(C_{AO} - C_{Ae}) \tag{3}$$

$$dx_A/d\theta = k_n(1 - x_A)^n \tag{4}$$

$$\text{where,} \quad k_n = k_r(C_{AO} - C_{Ae})^{n-1} \tag{5}$$

In the nth-order rate equation of Eq.(4), k_n (min^{-1}) and n(−) are the rate parameters which can be obtained from the relationship of x_A vs. θ.

The sterilization and the drying of foods are examples in which the dominant factor is a physical phenomenon namely the heat and mass transfers. For the physical transformations under heat and mass transfers, Fourie's and Fick's equations may be used, respectively. These laws state that the heat and mass transfer rates are propotional to the transfer area and to the differences of temperatures and concentration, respectively, and that they are inversely proportional to the transfer length.

The shape, the surface area and the transfer length of the transforming foods are usually not constant and can not be measured with sufficient accuracy. Therefore, we assumed that the heat and mass transfer rates may be proportional to only the nth-order values of the differences in temperature and concentration respectively, as follows :

$$dt/d\theta = k_h|t_e - t|^n \tag{6}$$

$$dy/d\theta = k_m|y_e - y|^n \tag{7}$$

where, t(°C) and y(example unit : g) are the temperature and the mass and so on at transforming time θ (min), and the subscript e is equilibrium state. k_n($°C^{1-n} \cdot \text{min}^{-1}$), k_m (example unit: $g^{1-n} \cdot \text{min}^{-1}$) and n (−) are the rate parameters which can be obtained.

Then, using a transforming ratio expressed by Eqs.(8) and (9), the rate equation is expressed by the nth-order rate equation just as in Eq.(4).

$$x_t = |(t - t_o)/(t_e - t_o)| \tag{8}$$

$$x_y = |(y - y_o)/(y_e - y_o)| \tag{9}$$

From Eqs.(4), (6) (9), we obtain:

$$k_n = k_h|t_e - t_o|^{n-1} \tag{10}$$

$$k_n = k_m|y_e - y_o|^{n-1} \tag{11}$$

The transforming ratios expressed as Eqs.(3), (8) and (9) are the dimentionless values which vary from 0 to 1 with the changes of $C_A = C_{AO} \rightarrow C_{Ae}$, $t = t_0 \rightarrow t_e$ and $y = y_0 \rightarrow y_e$, respectively. This value is convenient as being imdependent of the measuring properties, and of the unit and initial and equilibrium values, and so on.

When the relationship between the transforming ratio x_A and the transforming time θ

show a monotonous curve, the nth-order rate equation of Eq.(4) is useful simple rate equation.

2. Other-shape rate equations :

For the chemical, biological and physical transformations of foods, the relationship between the transforming ratio and the transforming time show often a S-shape curve or an other-shape one. The simple reaction mechanisms and the rate equations are as follows :

Other-shape model A :

For a reaction of autocatalitic type which can be seen with a bromination of acetone and so on, we can obtain the following S-shape rate equation.

$$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} R + S \tag{12}$$

$$\theta = 0 : C_A = C_{AO},\ C_B = C_{BO},\ C_S = C_{SO} \text{ and } C_R = 0$$

where, the product component S is a catalyst.

On the reaction of Eq.(12) : If the component B is in larger excess compared to the component A, and to the assumed constant in the progress of reaction, the rate equation is as follows. For the sake of simplification we provide that the reverse reaction is negligible and that the order of the forward reaction is in first order with respect to component A.

$$-dC_A/d\theta = k_1 C_A (C_{SO} + C_S) \tag{13}$$

In Eq.(13), if the transforming ratio x_A is expresed by Eq.(3), we obtain $C_A = C_{AO}(1-x_A)$, $C_S = C_{AO}x_A$. The rate equation is then obtained as follows :

$$dx_A/d\theta = k_\alpha (1 - x_A)(x_A + \alpha) \tag{14}$$

$$\text{where, } \quad k_\alpha = k_1 c_{AO} \tag{15}$$

$$\alpha = C_{SO}/C_{AO} \tag{16}$$

The rate equation of Eq.(14) is a useful simple rate equation especially when the relationship between the transforming ratio x_A and the transforming time θ show a S-shape curve. This equation is similar to the logistic curve equation which is well known as the one of the growth curve.

Other-shape model B :

For a reaction type which can show a enzyme reaction, we may obtain an other-shape rate equation.

$$A + S \underset{k_2}{\overset{k_1}{\rightleftarrows}} X, \qquad X \underset{k_4}{\overset{k_3}{\rightleftarrows}} R + S \tag{17), (18}$$

$$\theta = 0 : C_A = C_{AO},\ C_R = 0 \text{ and } C_S = C_{SO}$$

where, the components A, R and S are reactant, product and enzyme, respectively. The component X being an intermediate product rection of A with S, we can provide $C_{SO} = C_S + C_X$.

On the reactions Eqs.(17) and (18) : If we postulate simplifying that the reaction of R with S be negligible and the orders of the other reactions be in first order respect to each components, the following rate equation may be obtained, by using the quasi steady state method or the rate controlling step method.

$$-dC_A/d\theta = k_A C_A/(C_A + k_B) \tag{19}$$

where, $k_A = k_3 C_{SO}$ (19)

$$k_B = (k_2 + k_3)/k_1 \quad \text{or} \quad k_2/k_1 \tag{20), (21}$$

This formula is well known as the Michaelis-Mentein's equation, and k_B is called the Michaelis constant.

In Eq.(19), if the transforming ratio x_A is expressed by Eq. (3), the rate equation is obtained as follows :

$$dx_A/d\theta = k_\beta (1 - x_A)/(\beta - x_A) \tag{22}$$

where, $k_\beta = k_A/C_{AO}$ (23)

$$\beta = (k_B + C_{AO})/C_{AO} \tag{24}$$

The rate equation of Eq.(22) is useful for other-shape curve data, too.

Other-shape model C :

By a cosecutive reaction, we can obtain a S-shape rate equation too.

$$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} B \underset{k_4}{\overset{k_2}{\rightleftharpoons}} R \tag{25}$$

$\theta = 0$: $C_A = C_{AO}$, $C_B = 0$ and $C_R = 0$

On the reactions of Eq.(25) : If we postulate simplifying that the two reverse reactions are negligible and the orders of the forward reactions are first order, the rate equations become as follows :

$$-dC_A/d\theta = k_1 C_A \tag{26}$$

$$dC_B/d\theta = k_1 C_A - k_2 C_B \tag{27}$$

$$dC_R/d\theta = k_2 C_B \tag{28}$$

In Eqs.(26)~(28); if the transforming ratios x_A are expressed by Eq.(3), and x_B and x_R are respective components B and R are expressed by Eqs.(29) and (30), the rate equations are obtained as Eqs.(31)~(33).

$$x_B = C_B/C_{AO}, \quad x_R = C_R/C_{AO} \tag{29), (30}$$

$$dx_A/d\theta = k_1(1-x_A) \tag{31}$$

$$dx_B/d\theta = k_1(1-x_A) - k_2 x_B \tag{32}$$

$$dx_R/d\theta = k_2 x_B \tag{33}$$

where, x_B and X_R are the dimensionless value which may vary from 0 to 1 with the changes of $C_B = 0 \rightarrow C_{AO}$, $C_R = 0 \rightarrow C_{AO}$, respectively.

In Eqs.(31)~(33), the relationship between x_R vs. θ shows a S-shape curve. This model is not suitable for the simple S-shape rate equation for reason that the calculation of the simultaneous differential equations is too complicated. However, when the chemical, biological and physical transformations of foods proceed consecutively and the components or properties of the product R are prevalent, we must make use of this model.

If the reaction mechanism or physical phenomenon is elucidated even slightly, we should consider the rate equation based on the pseudo mechanism insted of the empirical rate equation described in the previous paper[1].

CALCULATION METHODS OF PARAMETERS

1. Method for differential data

When the experimental data are obtained as the differential data of $dx/d\theta$ vs. x, the rate parameter k, n and so on in various rate equations may be calculated by a linear least square method [2] using the following deformed equations.

For nth-order rate equation (Eq.(4)) :

$$\log(dx_A/d\theta) = \log k_n + n \log(1-x_A) \tag{34}$$

For other-shape rate equations ;

Model A (Eq.(14)) :

$$dx_A/d\theta = \alpha k_\alpha + (1-\alpha) k_\alpha x_A - k_\alpha x_A^2 \tag{35}$$

Model B (Eq.(22)) :

$$dx_A/d\theta = (k_\beta/\beta)(1-x_A) + (1/\beta) x_A (dx_A/d\theta) \tag{36}$$

Model C (Eqs.(31)~(33)) :

$$dx_A/d\theta = k_1(1-x_A), \quad dx_R/d\theta = k_2 x_B \tag{31), (33}$$

However, if the data are obtained as the integral data of x vs, θ, these method in general proves to be no better than the following method. The reason for this deficiency is that the derivative values of $dx/d\theta$ cannot be obtained reliably from the data x vs. θ.

2. Method for integral data

The experimental data are generally obtained as being the integral data of x vs. θ, because they data can be obtained in a more reliable way from the integral apparatuses

than from the differential ones.

If the rate equation can be analytically integrated, it becomes possible to obtain simply the rate parameters. The integrated equations for nth-order and other-shape simple rate equations assumed in this paper can be obtained as in the following equations:

For nth-order rate equations:

$n = 1$:

$$k_{n=1} = -(\ln(1 - x_A))/\theta \tag{37}$$

$$x_A = 1 - \exp(-k_{n=1}\,\theta) \tag{38}$$

$n \neq 1$:

$$k_n = ((1/(1 - x_A))^{n-1} - 1)/(n-1)\theta \tag{39}$$

$$x_A = 1 - (1 + k_n\,\theta\,(n-1))^{1/(1-n)} \tag{40}$$

For other-shape rate equations ;

Model A :

$$k_\alpha = (1/(1+\alpha))\ln((x_A + \alpha)/(1 - x_A)\,\alpha) \tag{41}$$

$$x_A = \alpha(X-1)/(\alpha X + 1) \tag{42}$$

where, $X = \exp((1+\alpha)\,k_\alpha\,\theta)$

Model B :

$$k_\beta = (x_A - (\beta - 1)\ln(1 - x_A))/\theta \tag{43}$$

x_A = a trial-and-error method is required

Model C :

$$k_1 = -(\ln(1 - x_A))/\theta \tag{44}$$

k_2 = a trial-and-error method is required

$$x_A = 1 - \exp(-k_1\,\theta) \tag{45}$$

$k_1 = k_2$:

$$x_B = k_1\,\theta\,\exp(-k_1\,\theta) \tag{46}$$

$$x_R = 1 - (1 + k_1\,\theta)\exp(-k_1\,\theta) \tag{47}$$

$k_1 \neq k_2$:

$$x_B = (k_1/(k_2 - k_1))X - (k_1/(k_2 - k_1))Y \tag{48}$$

$$x_R = x_A - x_B = 1 - (k_2/(k_2 - k_1))X + (k_1/(k_2 - k_1))Y \tag{49}$$

where, $X = \exp(-k_1\,\theta)$, $Y = \exp(-k_2\,\theta)$

In the nth-order rate equation, we must take for granted the value of n, and check the agreement of the various values of k_n. In the other-shape rate equation of model C, we must calculate the rate parameter k_2 by using a trial-and-error method.

When the data show considerable scattering, this method is in general not more helpful than the following numerical integral method.

When the rate equation is complicated and can not be analytically integrated, we must use the following numerical integral analysis too.

3. The method using numerical integration

The calculation method using numerical integration is very useful for various transforming rate equations. In this method, we use a non-linear least square method by means of a digital electric computer. The flow chart and the programs are the same as in the previous paper[1]. In this present paper, we used this method, and a "HITAC 8700–OS7" in the Computation Center of Hiroshima University.

BASIC CALCULATIONS FOR INFERENCES

If the true transforming mechanism is known as shown in the former section, we can obtain the ideal rate equation. However, the transforming mechanisms of foods are generally very complex. So we should infer pseudo transforming mechanisms. In this section, we elucidate a concrete case in which we used the inference of pseudo mechanisms.

In the previous paper[1], we have investigated the determination of the simple empirical rate equation as follows :

$$dx/d\theta = k_{n,\alpha}(1-x)^n(x+\alpha) \tag{50}$$

From the data calculated in Eqs.(4), (14), (22) and (31)~(33) which all have known mechanisms, the rate parameters $k_{n,\alpha}$, n and α in Eq.(50) may be calculated. The results are shown in Table 1. The estimated data in each run were given at the experimental points of x = 0.05, 0.1, 0.2, . . . 0.8, 0.9, 0.95 (–) as shown in the previous paper[1]. The number of data points was eleven. The standard deviation σ (–) in Table 1 is as follows :

Table 1. Rate parameters in Eq.(50) for estimated data with known mechanism

Data given by Eq.(4)		Rate parameters in Eq. (50)			Standard deviation
n (–)	k_n (min^{-1})	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)
2.0	0.60	0.238	2.40	2.18	0.00561
2.0	0.40	0.185	2.03	2.21	0.00625
1.5	0.25	0.138	1.65	1.73	0.00682
1.5	0.15	0.0923	1.46	1.75	0.00805
1.0	0.10	0.0753	1.16	1.29	0.0105
1.0	0.06	0.0474	1.08	1.30	0.0135
0.7	0.06	0.0529	0.961	1.03	0.0151
0.7	0.04	0.0349	0.965	1.02	0.0169
0.5	0.05	0.0492	0.850	0.857	0.0171
0.5	0.03	0.0302	0.817	0.862	0.0197
0.3	0.04	0.0445	0.737	0.694	0.0197
0.3	0.025	0.0280	0.719	0.691	0.0230

0.1	0.035	0.0469	0.594	0.558	0.0216
0.1	0.02	0.0281	0.551	0.572	0.0267
0.01	0.03	0.0416	0.568	0.477	0.0240
0.01	0.02	0.0313	0.486	0.527	0.0275

Data given by Eq.(4)		Rate parameters in Eq. (50)			Standard
α	k_α	$k_{n,\alpha}$	α	n	deviation
(–)	(min^{-1})	(min^{-1})	(–)	(–)	σ (–)
1.0	0.06	0.0573	1.05	0.987	0.000468
1.0	0.04	0.0403	0.992	1.00	0.000401
0.5	0.10	0.0981	0.511	0.993	0.000463
0.5	0.06	0.0606	0.495	1.00	0.000270
0.1	0.15	0.151	0.0986	1.00	0.00101
0.1	0.10	0.100	0.0999	1.00	0.000575
0.01	0.25	0.245	0.0107	0.983	0.00320
0.01	0.15	0.148	0.0103	0.986	0.00268
0.001	0.30	0.299	0.00101	0.994	0.00130
0.001	0.20	0.201	0.000962	1.00	0.000537

Data given by Eq. (22)		Rate parameters in Eq. (50)			Standard
β	$k\beta$	$k_{n,\alpha}$	α	n	deviation
(–)	(min^{-1})	(min^{-1})	(–)	(–)	σ (–)
1.1	0.04	0.0430	0.717	0.607	0.159
1.1	0.025	0.0291	0.646	0.634	0.0197
1.2	0.05	0.0415	0.889	0.681	0.0134
1.2	0.03	0.0266	0.814	0.701	0.0164
1.5	0.08	0.0512	0.940	0.879	0.00994
1.5	0.05	0.0296	1.02	0.857	0.0111
2.0	0.12	0.0510	1.07	1.00	0.00971
2.0	0.08	0.0345	1.04	1.00	0.0111
10.0	0.90	0.0607	1.32	1.21	0.0113
10.0	0.55	0.0441	1.07	1.23	0.0117

Data by Eqs.(31)~(33)		Rate parameters in Eq. (50)			Standard
k_2/k_1	k_1	$k_{n,\alpha}$	α	n	deviation
(–)	(min^{-1})	(min^{-1})	(–)	(–)	σ (–)
1.0	0.15	0.205	0.117	1.33	0.00924
1.0	0.10	0.137	0.116	1.33	0.00920
5.0	0.10	0.227	0.162	1.51	0.0105
5.0	0.06	0.136	0.163	1.50	0.0106
10.0	0.10	0.173	0.323	1.42	0.0102
10.0	0.06	0.104	0.324	1.42	0.0103
100.0	0.10	0.0770	1.11	1.28	0.00957
100.0	0.06	0.0498	1.01	1.30	0.0115

$$\sigma = \sum_{i=1}^{N} \{(x_{obs} - x_{cal})_i^2 / N\}^{1/2} \tag{51}$$

where, x_{obs} and x_{cal} are the data and calculated values of x, and N is the total number of the experimental points.

The obtained values of α and n are particulary interesting, because these values indicate the form of various curves. The relationships between the rate parameters α and n in Eq.(50) are shown in Fig. 1. In Fig. 1, it seems that the relationships are less affected bv the values of $k_{n,\alpha}$. The points for the various foods are in the examples as will be shown latter.

If we calculate the parameters α and n in Eq.(50) on the unknown various transformations of foods, we can infer the pseudo transforming mechanisms by using Fig. 1 which have the relationships of the various mechanisms known.

EXAMPLES OF INFERENCES

As data of examples of inferences we may use the soaking and cooking data of soybean[4], red bean[5], the cooking data of potato[6], sweet potato[6], carrot[7], radish[7] and so on. The results obtained this way are shown in the left half part of Table 2. A part of the typical results is shown also in Fig. 1. By using the results of Fig. 1, the inference of the pseudo transforming mechanisms of example data in very difficult, because the points show considerable scattering. However, it may be cocluded that the soaking mechanisms of soybean are probably related to the nth-order model or other-shape model B and that the cooking mechanisms of soybean are probably related to the other-shape model A.

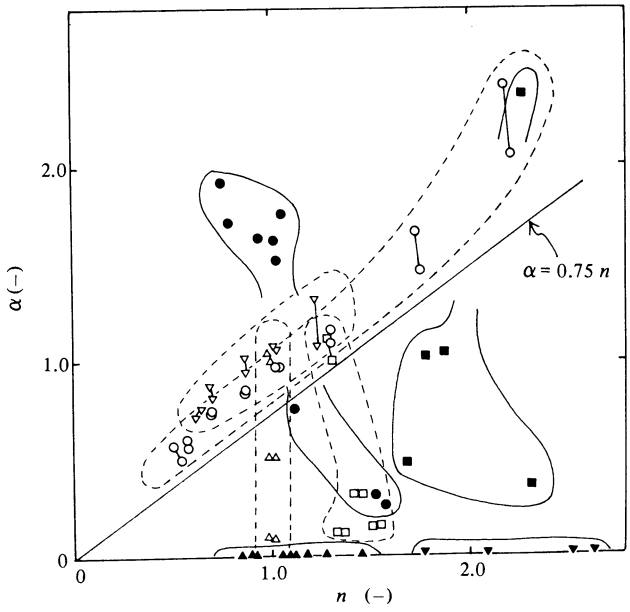

Fig. 1. Relationships between the rate parameters α and n in Eq. (50)
nth-order model (Eq. (4)) : ○
Other shape model A (Eq. (14)) : △
Other shape model B (Eq. (22)) : ▽
Other shape model C (Eqs. (31) ~ (33)) : □
Example data :
Soybean[4] : ● Red bean[5] : ▲
Carrot[7] : ■ Radish[7] : ▼

In the cooking of carrot and radish, the value of n is neary 2.0 and the mechanism is not related to the nth-order model. So, we must introduce the S-shape empirical model which has the various values of n as examined in the previous paper[1]. In Fig. 1, we may conclude that the upper parts of the solid line of $\alpha = 0.75n$ are related to the nth-order empirical model and that the below parts are related to the S-shape empirical model by Eq. (50).

From these considerations, the determination method of the empirical rate equation in the previous paper[1] becomes modified as follows.

First step calculation :

calculation of $k_{n,\alpha}$, α and n in Eq. (50)

Next step calculations :

For $\alpha \geqq 0.75n$, nth-order model ;

calculation of k_n and n in Eq.(4),

and fixing n = 0.01, 0.1, 0.3, 0.5, 0.7, 1.0, 1.3, 1.5, 1.7 or 2.0

For $\alpha < 0.75n$, S-shape model ;

fixing α = 1.3, 1.0, 0.7, 0.5, 0.3, 0.1, 0.05, 0.03, 0.01, 0.005 or 0.001 for n = 0.5, 1.0, 1.5 or 2.0, respectively

The results become by the modified method are shown in the right half part of Table 2.

Table 2. Rate parameters in Eq. (50) for example data [4–7]

Soybean (Data by Kubota [4])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=0.7}$ (min^{-1})	σ (–)
100	0.0887	0.329	1.51	0.0229	0.0364	0.0387
90	0.135	0.258	1.57	0.0352	0.0477	0.0536
80	0.0432	0.753	1.11	0.0294	0.0375	0.0332
70	0.0153	1.91	0.750	0.0533	0.0351	0.0521
60	0.0129	1.70	0.796	0.0320	0.0255	0.0333
50	0.00860	1.62	1.01	0.0238	0.0144	0.0254
40	0.00556	1.52	1.02	0.0244	0.00870	0.0278
30	0.00351	1.75	1.05	0.0279	0.00616	0.0315
20	0.00186	1.63	0.941	0.0230	0.00328	0.0220

Red bean (Data by Kubota [5])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=1.0,\alpha=0.03}$ (min^{-1})	σ (–)
97	0.0928	0.0880	1.16	0.0256	0.126	0.0583
90	0.139	0.0253	1.45	0.0255	0.116	0.0465
80	0.104	0.00980	1.09	0.0207	0.0774	0.0360
70	0.0589	0.0121	0.844	0.0177	0.0490	0.0506
60	0.0361	0.0113	0.870	0.00913	0.0294	0.0491
50	0.0280	0.00536	0.898	0.00673	0.0194	0.0662
40	0.0197	0.00387	1.06	0.0162	0.0121	0.0592
30	0.0134	0.00285	1.26	0.00876	0.00761	0.0497
20	0.00735	0.00273	1.06	0.00555	0.00436	0.0684

Potato (Data by Kubota [6])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=1.0,\alpha=1.0}$ (min^{-1})	σ (–)
99.5	0.161	1.18	1.54	0.0416	0.138	0.0624
95	0.580	0.00238	1.70	0.0349	0.0452	0.143
90	0.128	0.110	0.891	0.0433	0.0360	0.0947
85	0.0214	0.780	0.710	0.0652	0.0208	0.0707
80	0.0118	0.959	0.580	0.0747	0.0144	0.0727

Sweet potato (Data by Kubota [6])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=1.5,\alpha=0.03}$ (min^{-1})	σ (–)
99.5	1.99	0.0195	1.92	0.0185	1.51	0.0389
95	1.21	0.00985	1.72	0.0385	0.874	0.0419
90	0.817	0.000174	2.11	0.0239	0.312	0.0669
85	0.132	0.0432	1.17	0.0349	0.162	0.0402
80	0.226	0.0150	1.83	0.0551	0.175	0.0579

Carrot (Data by Takasaki [7])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=2.0,\alpha=1.3}$ (min^{-1})	σ (–)
99.5	0.136	2.36	2.27	0.0473	0.198	0.0541
95	0.175	0.484	1.67	0.0232	0.101	0.0491
90	0.133	0.352	2.30	0.0217	0.0461	0.0247
85	0.0361	1.03	1.86	0.0337	0.0335	0.0349
80	0.0209	1.02	1.77	0.0422	0.0200	0.0434

Radish (Data by Takasaki [7])

t (°C)	$k_{n,\alpha}$ (min^{-1})	α (–)	n (–)	σ (–)	$k_{n=2.0,\alpha=0.03}$ (min^{-1})	σ (–)
99.5	0.729	0.0192	2.50	0.0402	0.550	0.0497
95	0.756	0.00155	2.86	0.0469	0.344	0.0588
90	0.194	0.0559	2.09	0.0488	0.228	0.0545
85	0.343	0.000340	2.61	0.0356	0.141	0.0637
80	0.0786	0.0112	1.76	0.0333	0.0645	0.0505

If the data of x vs. θ are not scattered and are obtained with reliability, we may infer the pseudo transforming mechanisms of foods by using the relationships between the transforming time ratio and the parameters of various models as shown in Figs. 2~4, too. In Figs. 2~4, $\theta_{x=0.5}$ is the transforming time at $x = 0.5$. In this method, we must assume various models, and check the agreement of the values of obtained parameters.

This paper was presented in part at the Food Chemical Engineering Symposium in the 13th Autumn Meeting of the Society of Chemical Engineers, Japan (October 20, 1979; Nagoya).

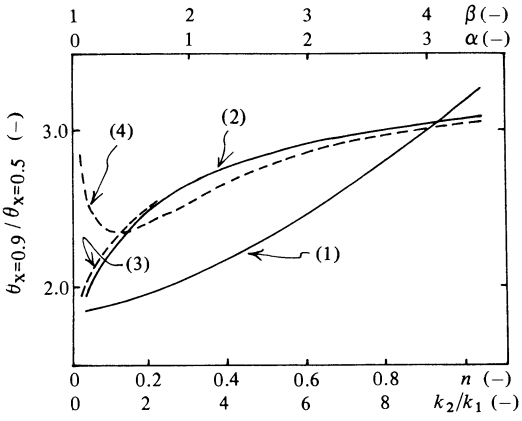

Fig. 2. Relationships between the transforming time ratio and the rate parameters on the various known models.

nth-order model (Eq. (4)) : curve (1)
Other shape models A, B, C : curves (2), (3), (4) (Eqs. (14), (22), (31)~(33))

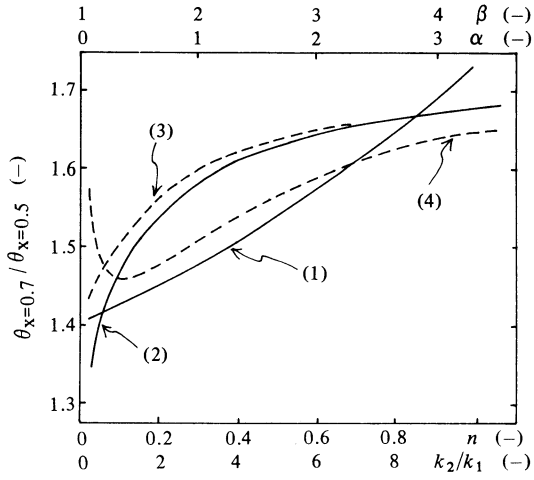

Fig. 3. Relationships between the transforming time ratio and the rate parameters on the various known models.

nth-order model (Eq.(4)) : curve (1)
Other shape models A, B, C : curves (2), (3), (4) (Eqs.(14), (22), (31) ~ (33))

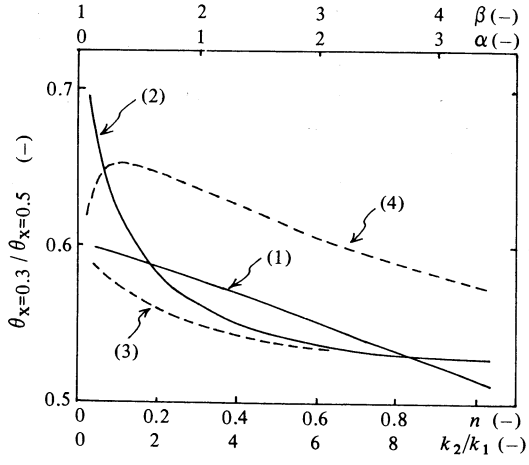

Fig. 4. Relationships between the transforming time ratio and the rate parameters on the various known models.

nth-order model (Eq.(4)) : curve (1)
Other shape models A, B, C : curves (2), (3), (4) (Eqs.(14), (22), (31) ~ (33))

SUMMARY

In a former paper[1], we studied the determination of the following simple empirical rate equation for the various transformations of foods.

$$dx/d\theta = k_{n,\alpha}(1-x)^n(x+\alpha)$$

where, x (−) and θ (min) are the transforming ratio and time, respectively, and $k_{n,\alpha}$, α and n are the rate parameters which can be obtained from experimental data.

This time, we took up the inference of the pseudo transforming mechanisms using this simple empirical rate equation. The relationships between the rate parameters α and n have been shown on the assumed various mechanisms, and by using these relationships we attempted to infer the cooking pseudo mechanisms of various foods. The pseudo mechanisms infered in this paper is very helpful to find real mechanisms.

NOTATIONS

C_j : concentration of j-th component, (g-mol/cm^3)

k_n, k_α, k_β, k_1, k_2 and $k_{n,\alpha}$:
rate parameters in Eqs.(4), (14), (22), (31)~(33) and (50), (min^{-1})

n : rate parameter in Eqs.(2) and (50), (−)

x : transforming ratio by Eqs.(3), (8) and (9), (−)

α : rate parameter in Eqs.(14) and (50), (−)

β : rate parameter in Eq.(22), (−)

θ : transforming time, (min)

σ : standard deviation by Eq.(51), (−)

Subscripts ;

0 and e : initial and equilibrium states

obs and cal : observed and calculated values

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簡単な速度式を用いた食品の擬似処理機構の推察

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前報[1]において，食品の各種処理における簡単な経験的速度式の設定について研究した。

$$dx/d\theta = k_{n,\alpha}(1-x)^n(x+\alpha)$$

ここで，x（－），θ（min）は，それぞれ処理率，処理時間，また，$k_{n,\alpha}$，n および α は，実験データから得られる速度パラメータである。

本報では，この簡単な経験的速度式を用いて，擬似処理機構を推察する研究を行なった。速度パラメータ α 対 n の関係を利用して，各種食品のクッキングの擬似機構の推察を試みた。本研究で推察して得られる擬似処理機構は，真の機構を見出していくのに役立つものと考えられる。